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The capacitance transient spectroscopic technique is described along with the major variations in the techniques depending on the particular instrumentation used to process the capacitance transient. Expressions for the theoretical line shape are derived for the lock-in amplifier version of the technique with arbitrary phase setting. The results show excellent agreement with experimental spectra. Expressions are derived which are useful in determining defect level parameters from a single spectrum, rather than from an
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20. Abstract (Continued)

Arrhenius plot from a series of spectra. A computer program is given for plotting theoretical spectra, which is useful for determining the effects of defect level parameters on spectra and for unfolding complex spectra.

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Illustrations

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Lineshape Analysis for Capacitance Transient Spectra

I. INTRODUCTION

Capacitance transient spectroscopy has, in recent years, gained widespread use in the detection and study of defect states in semiconductor materials and devices.[1] The technique was originally developed by Lang[2] and called deep-level transient spectroscopy (DLTS). Major variations on the technique have been developed by Kimerling[3] and Miller et al.[4]

The technique is based on the work of Williams[5] and Sah et al[6] where a transient is produced in the capacitance of a diode structure, following a sudden bias increase, and resulting from charge carrier emission from defects in the depletion region. Determination of the decay-time constant, τ, of the capacitance transient as a function of temperature yields important information about the defect centers.

(Received for publication 1 November 1979)

1. Miller, G. L., Lang, D. V., and Kimerling, L. C. (1977) Ann. Rev. Mat. Sci. 1977:377.
2. Lang, D. V. (1974) J. Appl. Phys. 45:3023.
3. Kimerling, L. C. (1977) Radiation effects in semiconductors - 1976, Inst. of Physics Conf. Series No. 31, 221.
4. Miller, G. L., Ramirez, J. V., and Robinson, D. A. H. (1975) J. Appl. Phys. 46:2638.
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6. Sah, C. T., Forbes, L., Rosier, L. L., and Tasch, Jr., A. F. (1970) Solid-State Electron. 13:759.

In capacitance transient spectroscopy, periodic bias pulses are used to produce a repetitive train of capacitance transients. This signal is then processed by some apparatus which has a peak response for a particular τ. As the temperature of the sample is varied, a peak in the output of this apparatus will be recorded each time the emission-time constant of a defect matches that to which the instrument is tuned. The lineshape of the spectra which are obtained depend on the particular apparatus used to process the capacitance transient signal. Lang[2] used a double boxcar integrator. Kimerling[3] uses a lock-in amplifier. Miller[4] uses an exponential correlator. The paper by Miller et al[4] gives the lineshape for the double boxcar and exponential correlator, and also for one particular phase setting of a lock-in amplifier.

Different phase settings are possible when using a lock-in amplifier due to the way it processes the capacitance transient signal. The tuned amplifiers of the input channel allow only the fundamental Fourier component of the signal to pass. The mixer then passes the signal unaltered for a half cycle and inverts the next half cycle. It is the phase of this operation which is adjustable. Finally, the output filters smooth this out to a D.C. average output. The phase of the fundamental Fourier component is not constant in our case, since as temperature is varied, the time constant of the exponential decay varies, resulting in a variation of the phase of the signal reaching the lock-in mixer.

If the mixer operation phase is set to coincide with the beginning of the capacitance transient (end of the bias pulse) then one gets the lineshape reported by Miller et al.[4] However, if the phase is set to be in phase with the fundamental Fourier component at that temperature for which it has maximum amplitude, then a different lineshape is generated. Some lock-in amplifiers have a phase independent (vector amplitude) output which gives still another lineshape.

In previous work[7, 8] we have used the second mentioned phase setting, choosing to be in phase with the fundamental Fourier component at maximum amplitude of this component. This has been shown[9] to require a phase setting of 24.5° before the bias pulse (beginning of transient). This phase setting is convenient since one can monitor the mixer output during a run and verify that the in-phase point occurs at the peak in the output. This gives assurance that the lock-in amplifier has been properly tuned and has not drifted, which can be a concern at very low frequencies (down to 0.2 Hz).

7. Drevinsky, P.J., Schott, J.T., DeAngelis, H.M., Kirkpatrick, A.R., and Minnucci, J.A. (1979) Conf. Record of the Thirteenth IEEE Photovoltaics Specialists Conference - 1978, 1232.

8. Schott, J.T., DeAngelis, H.M., and Drevinsky, P.J. (1980) J. Electron. Mat., to be published.

9. Schott, J.T., DeAngelis, H.M., and White, W.R. (1976) Air Force Technical Report, AFCRL-TR-76-0024.

In a previous report[9] we derived the expressions necessary to relate lock-in amplifier frequency to emission time constant and peak height to defect concentration, for this phase setting. Each time a spectrum at a different frequency is generated, another time constant/temperature data point for an Arrhenius plot which will yield the basic defect paramete ؞ is received. However, this only uses one point of each spectrum, namely, the peak position. The rest of the lineshape contains information about the emission time constant at other temperatures as well. In fact a single spectrum at a single frequency contains all the information necessary to obtain the parameters received from an Arrhenius plot using a number of spectra at different frequencies.

In this report, we derive the theoretical lineshape for arbitrary lock-in amplifier phase, and the expressions necessary to extract information from these spectra. Theoretical curves are compared with experimental spectra. An appendix gives a computer program to generate theoretical capacitance transient spectra.

2. SIMPLIFIED LOCK-IN AMPLIFIER TREATMENT

A simplified view of lock-in amplifier operation is to consider it to act as a correlator with a sine wave weighting function. This is the view taken by Miller et al[4] in comparing the lock-in approach with their exponential correlator approach. Then for a capacitance signal of the form exp $(-t/\tau)$, we get a lock-in response of the form

$$A = \frac{1}{L}\int_0^L e^{-t/\tau} \sin \frac{2\pi t}{L}\, dt \tag{1}$$

$$= \frac{2\pi(1 - e^{-L/\tau})}{\frac{L^2}{\tau^2} + 4\pi^2} \tag{2}$$

where the lock-in amplifier is tuned to a frequency, $F = 1/L$. If we define a dimensionless parameter, α, such that

$$\alpha = \frac{\tau}{L} = \tau F \tag{3}$$

we then get the lineshape expression

$$A(\alpha) = \frac{2\pi\alpha^2(1 - e^{-1/\alpha})}{4\pi^2\alpha^2 + 1} \tag{4}$$

Of course A is implicitly a function of temperature T, through the standard emission rate equation

$$\alpha = \tau F = F \frac{e^{\Delta E/kT}}{\sigma\langle v\rangle N} \tag{5}$$

where k is the Boltzmann constant, σ is the defect capture cross section, $\langle v\rangle$ is the carrier thermal velocity, and N is the density of states of the appropriate band. This lineshape is the one reported by Miller et al[4] for Kimerling's lock-in amplifier spectra.

3. MORE EXACT TREATMENT FOR 0° PHASE

For a more careful treatment, we must consider the complete sequence of input channel filtering, mixing, and output channel filtering. The effect of the tuned amplifiers of the input channel is to pass only the fundamental Fourier component of the exponential train. In a previous report,[9] we showed this Fourier component to be

$$F(t) = a_1 \cos \frac{2\pi t}{L} + b_1 \sin \frac{2\pi t}{L} \tag{6}$$

$$= c_1 \sin \left(\frac{2\pi t}{L} + \tan^{-1}\frac{a_1}{b_1}\right) \tag{7}$$

where

$$a_1 = \frac{2\alpha(e^{-1/\alpha} - 1)}{(4\pi^2\alpha^2 + 1)} \tag{8}$$

$$b_1 = \frac{4\pi\alpha^2(e^{-1/\alpha} - 1)}{(4\pi^2\alpha^2 + 1)} \tag{9}$$

$$c_1 = \frac{2\alpha(e^{-1/\alpha} - 1)}{(4\pi^2\alpha^2 + 1)^{1/2}} \tag{10}$$

$$\frac{a_1}{b_1} = \frac{1}{2\pi\alpha} \tag{11}$$

The effect of the mixer operation and the averaging of the output channel filters can then be given by

$$A = \frac{1}{L}\int_{-L/2}^{0} F(t)\,dt - \frac{1}{L}\int_{0}^{L/2} F(t)\,dt \tag{12}$$

provided the phase of the mixer operation is set to 0 degrees with respect to the beginning of the capacitance transient. Substituting for the Fourier component using Eq. (6), we find that the cosine term averages to zero, and we are left with

$$A(\alpha) = b_1 \left\{ \frac{1}{L}\int_{-L/2}^{0} \sin\frac{2\pi t}{L}\,dt - \frac{1}{L}\int_{0}^{L/2} \sin\frac{2\pi t}{L}\,dt \right\}$$

$$= b_1 \left\{ -\frac{2}{\pi} \right\} = \frac{8\alpha^2(1 - e^{-1/\alpha})}{4\pi^2\alpha^2 + 1} \tag{13}$$

Note that this is of the same form as Eq. (4) found above, only differing by a constant factor.

4. LINESHAPE FOR ARBITRARY PHASE

The above lineshape is only correct for a particular phase setting of the lock-in amplifier. As mentioned in the introduction, however, other phase settings are sometimes convenient. If we consider the lock-in mixer operation phase to be set to an arbitrary angle ϕ ($0 \leq \phi \leq 2\pi$) before the beginning the capacitance transient, then the lock-in reponse will be given by

$$A = \frac{1}{L} \int_{(-L/2 - \phi L/2\pi)}^{-\phi L/2\pi} F(t)\, dt - \frac{1}{L} \int_{-\phi L/2\pi}^{(L/2 - \phi L/2\pi)} F(t)\, dt \tag{14}$$

Substituting for the Fourier component from Eq. (7) we have

$$A = c_1 \left\{ \frac{1}{L} \int_{(-L/2 - \phi L/2\pi)}^{-\phi L/2\pi} \sin\left(\frac{2\pi t}{L} + \tan^{-1} \frac{1}{2\pi\alpha}\right) dt \right.$$

$$\left. - \frac{1}{L} \int_{-\phi L/2\pi}^{(L/2 - \phi L/2\pi)} \sin\left(\frac{2\pi t}{L} + \tan^{-1} \frac{1}{2\pi\alpha}\right) dt \right\}$$

$$= c_1 \left\{ -\frac{2}{\pi} \cos\left(\tan^{-1} \frac{1}{2\pi\alpha} - \phi\right) \right\} \tag{15}$$

Thus, substituting Eq. (10), we have

$$A(\alpha) = \frac{4\alpha(1 - e^{-1/\alpha})}{\pi(4\pi^2\alpha^2 + 1)^{1/2}} \cos\left(\tan^{-1} \frac{1}{2\pi\alpha} - \phi\right) \tag{16}$$

We can now consider some special cases. For $\phi = 0$, we can construct a right triangle with two sides of length 1 and $2\pi\alpha$, and by calculating the hypotenuse, immediately find

$$\cos\left(\tan^{-1} \frac{1}{2\pi\alpha}\right) = \frac{2\pi\alpha}{(4\pi^2\alpha^2 + 1)^{1/2}} \tag{17}$$

Making this substitution, we get the lineshape of Eq. (13) found above.

In a previous report[9] we found the value of α, to be denoted α_{max}, for which the amplitude of the fundamental Fourier component (coefficient c_1 given by Eq. (10)), is a maximum. To be in phase with the Fourier component at its maximum amplitude, we must set the lock-in phase to

$$\phi = \tan^{-1} \frac{1}{2\pi\alpha_{max}} \cong 24.5^{\circ}$$

The lineshape is then

$$A(\alpha) = \frac{4\alpha(1 - e^{-1/\alpha})}{\pi(4\pi^2\alpha^2 + 1)^{1/2}} \cos\left(\tan^{-1} \frac{1}{2\pi\alpha} - 24.5^{\circ}\right) \tag{18}$$

This is the lineshape appropriate for all our published data.

If one has a lock-in amplifier which has a phase independent or vector amplitude output, then the lineshape is just the general form without the cosine factor

$$A(\alpha) = \frac{4\alpha(1 - e^{-1/\alpha})}{\pi(4\pi^2\alpha^2 + 1)^{1/2}} \tag{19}$$

Such instruments are really dual channel lock-in amplifiers with one channel output related to the cosine of the phase angle as above, and the other channel 90° out of phase and related to the sine of the phase angle. The phase independent or vector amplitude output is obtained from the sum of the squares of these two outputs.

Figure 1 shows a plot of each of the three lineshape equations plotted on a temperature scale appropriate for the thermocouple used in our experiments. The curves are generated by using Eq. (5) to determine the value of α for each temperature value, and then using the appropriate $A(\alpha)$ equation to determine the amplitude at that temperature. Figure 2 shows experimental spectra for two different phase settings. The agreement between theory and experiment is excellent.

5. DETERMINATION OF ACTIVATION ENERGY FROM LINESHAPE

In the introduction, it was pointed out that a single spectrum contains all the information necessary to determine the defect activation energy, provided more than just the peak maximum point is used. From Eq. (5) we can write

$$\alpha = C\, T^{-2}\, e^{\Delta E/kT} \tag{20}$$

where the T^{-2} dependence comes from the $T^{1/2}$ dependence of the thermal velocity and the $T^{3/2}$ dependence of the density of states and where we have assumed a temperature indpendent cross section. All other factors have been lumped into the

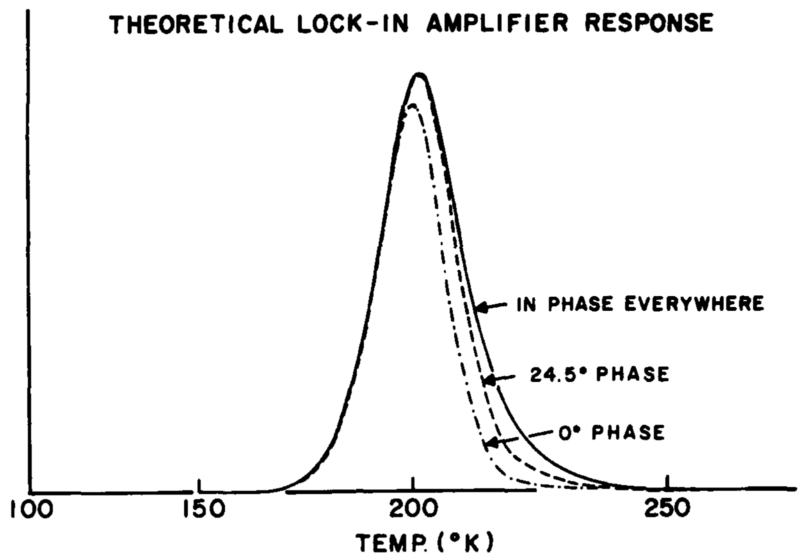

Figure 1. Theoretical Lineshapes for the Lock-In Amplifier Version of Capacitance Transient Spectroscopy for Different Lock-In Amplifier Phase Settings (Mixer 0° or 24.5° Before Beginning of Capacitance Transient) or for Phase Independent (Vector Amplitude) Output. The temperature scale is one appropriate for thermocouple output

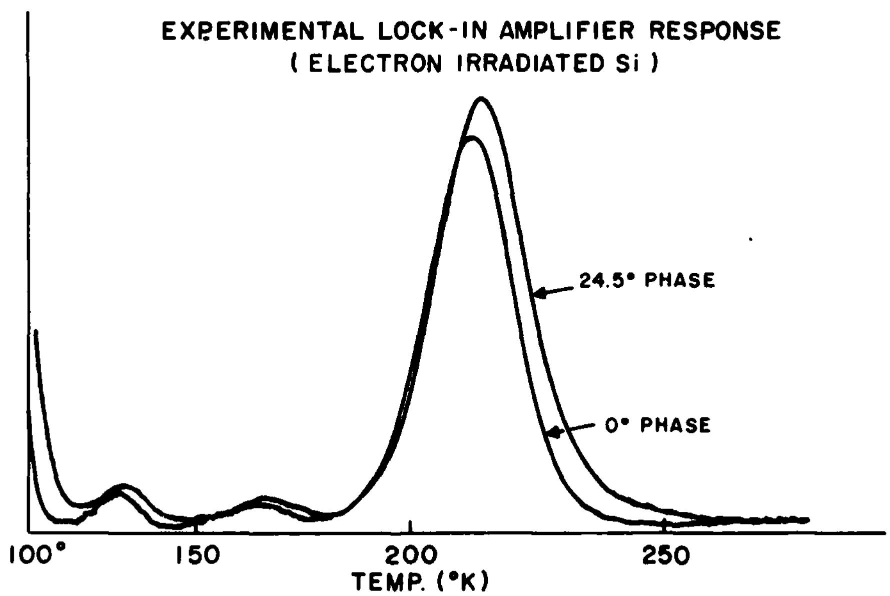

Figure 2. Experimental Spectra for the E-Center in Electron Irradiated Silicon for Two Lock-In Amplifier Phase Settings

constant C. We now choose two easily definable points on the lineshape curve $A(\alpha)$. For example, we might choose α_1 and α_2 such that $A(\alpha_1) = A(\alpha_2) \frac{1}{2} A_{max}$. From Eq. (20), there are two temperatures corresponding to the two α's which equally well define these half-maximum points. If $\alpha_1 < \alpha_2$ and $T_1 < T_2$, then α_1 corresponds to T_2 and α_2 corresponds to T_1, since large α means small T. We can thus write

$$\alpha_1 = C\, T_2^{-2}\, e^{\Delta E/kT_2} \tag{21}$$

and

$$\alpha_2 = C\, T_1^{-2}\, e^{\Delta E/kT_1} \tag{22}$$

Taking the natural logarithm of both equations, we get

$$\ln \alpha_1 = \ln C - 2 \ln T_2 + \frac{\Delta E}{kT_2} \tag{23}$$

$$\ln \alpha_2 = \ln C - 2 \ln T_1 + \frac{\Delta E}{kT_1} \tag{24}$$

Subtracting Eq. (23) from Eq. (24), we get

$$\ln \frac{\alpha_2}{\alpha_1} = \frac{\Delta E}{kT_1} - \frac{\Delta E}{kT_2} + 2 \ln \frac{T_2}{T_1} \tag{25}$$

or

$$\Delta E = \frac{k \ln \frac{\alpha_2}{\alpha_1}}{\frac{1}{T_1} - \frac{1}{T_2}} - 2k \left(\frac{\ln \frac{T_2}{T_1}}{\frac{1}{T_1} - \frac{1}{T_2}} \right) \tag{26}$$

If we use the approximation

$$\ln x \cong 2 \left(\frac{x - 1}{x + 1} \right) \tag{27}$$

for x not too far from unity, and if we write

$$T_2 = T_{av} + \Delta \tag{28}$$

$$T_1 = T_{av} - \Delta$$

where T_{av} is the average of T_1 and T_2, we find

$$\left(\frac{\ell n \frac{T_2}{T_1}}{\frac{1}{T_1} - \frac{1}{T_2}}\right) \cong T_{av} + \frac{\Delta^2}{T_{av}} \cong T_{av} \cong T_{max} \tag{29}$$

Equation (26) can then be written

$$\Delta E = \frac{k \,\ell n \frac{\alpha_2}{\alpha_1}}{\frac{1}{T_1} - \frac{1}{T_2}} - 2kT_{max} \tag{30}$$

This result has been derived by others for the 0^o phase lineshape.[10] As mentioned above, one need not use the half-maximum points. If one only had half the curve, for example, the one-half maximum point and the full maximum point could be used. If the left half of the curve (from a temperature viewpoint) were available, one could get the activation energy from

$$\Delta E = \frac{k \,\ell n \left(\frac{\alpha_2}{\alpha_{max}}\right)}{\frac{1}{T_1} - \frac{1}{T_{max}}} - 2kT_{max} \tag{31}$$

Errors due to noise in the experimentally determined lineshape are just compounded when the two points chosen are close together. It is advisable, therefore, to use the two half-maximum points.

In order to do all of this, the appropriate points on the experimental curves must be able to be accurately determined. This means that a good clean trace with an obvious baseline must be available. If there is a weak, noisy signal, or one whose baseline is not obvious, it is better to do an Arrhenius plot from a number of scans.

10. Kimerling, L.C., private communication.

Table 1 gives the parameters necessary to perform the above calculations for the various lock-in phase settings.

Table 1. Lineshape Expressions and Values of Parameters Defined in the Text, for Various Lock-In Amplifier Phase Settings

	0°	24.5°	Ph-ind.
$A(\alpha)$	$\frac{8\alpha^2(1-e^{-1/\alpha})}{4\pi^2\alpha^2+1}$	$\frac{4\alpha(1-e^{-1/\alpha})}{\pi(4\pi^2\alpha^2+1)^{1/2}}\cos(\tan^{-1}\frac{1}{2\pi\alpha}-\phi)$	$\frac{4\alpha(1-e^{-1/\alpha})}{\pi(4\pi^2\alpha^2+1)^{1/2}}$
α_{max}	0.4243	0.3485	0.3485
A_{max}	0.1608	0.1739	0.1739
$\frac{\text{sq. wave resp.}^*}{\text{exp. resp.}}$	2.52	2.33	2.33
α_1	0.1291	0.09657	0.07559
α_2	1.9613	1.643	1.775
$\frac{\alpha_2}{\alpha_1}$	15.19	17.01	23.48
$\frac{\alpha_2}{\alpha_{max}}$ †	4.622	4.715	5.093
$\frac{\alpha_{max}}{\alpha_1}$ ‡	3.286	3.609	4.610

*Ratio of unit square wave response (phase set for maximum response) to unit exponential train response (phase set to indicated value).

†For calculating activation energy from left hand side of peak lineshape.

‡For calculating activation energy from right hand side of peak lineshape.

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2. Lang, D.V. (1974) J. Appl. Phys. 45:3023.
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9. Schott, J.T., DeAngelis, H.M., and White, W.R. (1976) Air Force Technical Report, AFCRL-TR-76-0024.
10. Kimerling, L.C. private communication.

Appendix

Computer Plotted Spectra

The following program plots capacitance transient spectra, given the input of activation energy, effective cross section and amplitude for each level. The comment statements at the beginning of the program describe it more fully. It is written in Tektest III language for use with a Tektronix S-3260 integrated circuit test system.

To run the program, ensure that the proper disc (A65B Hanscom) is in operation. Then, after typing:

ctrl C

to obtain the executive prompter ($), type either:

DRIVE Ø

or:

DRIVE 1

followed by a carriage return (CR), depending on which drive contains the proper disc. Then type:

IDENT SCH

followed by a CR, and then:

RUN DLTS

followed by a CR. You then enter data as requested by the computer.

```
   1.0100 *              TRANSIENT CAPACITANCE SPECTROSCOPY
   1.0200 *                          WRITTEN BY
   1.0300 *                        JOHN T. SCHOTT
   1.0400 *                  (LATEST REVISION-FEB 79)
   1.0500 *
   1.0600 *  THIS PROGRAM PLOTS COMBINED AND INDIVIDUAL TRANSIENT CAPACITANCE
   1.0700 *  (DLTS) SPECTRA AND SUPERPOSITIONS OF THE TWO.  IT ASSUMES THE
   1.0800 *  USE OF A LOCK-IN AMPLIFIER WITH VARIOUS PHASE SETTING OPTIONS.
   1.0900 *  MATERIAL CONSTANTS CAN BE SET FOR EITHER N- OR P-TYPE SILICON
   1.1000 *  OR GALLIUM ARSENIDE.  TEMPERATURE IS PLOTTED ON A SCALE APPRO-
   1.1100 *  PRIATE FOR A COPPER-CONSTANTAN THERMOCOUPLE.  HARD COPY
   1.1200 *  IMAGE SIZE MAY BE ADJUSTED TO DUPLICATE SCALE OF EXPERIMENTAL
   1.1300 *  TRACES BY APPROPRIATE TEMPERATURE RANGE INPUT AND ADJUSTMENT
   1.1400 *  OF 'SCALE' VALUES.

   2.1000    SUBROUTINE DCOORD(4),SCOORD(4):GRAPHV
   2.2000    SUBROUTINE VECTRF(4),CURSOR(2),DRAWV(3):GRAPHV
   2.3000    ARRAY E(10),SIGMA(10),AMP(10)
   2.4000    ARRAY X(4),Y(4),S2(4)
   2.5000    ARRAY EI(10),SIGMAI(10),AMPI(10)
   2.6000    ARRAY EC(10),SIGMAC(10),AMPC(10)

   3.0100    PRESET X=-252.87,-195.802,0,100
   3.0200    PRESET Y=-6.197755,-5.535673,0,4.27961
   3.0300    PRESET S2=.241816E-3,.1355393E-3,.9026148E-4,.720794E-4
   3.0400    CONSTANT K=8.62E-5
   3.0500    CONSTANT PHASE=.4284029
   3.0600    CONSTANT PI=3.141593
   3.0700    CONSTANT C1=2E-22
   3.0800    CONSTANT C2=5E-22
   3.0900    CONSTANT C3=5E-21
   3.1000    CONSTANT C4=7E-22

   4.0010 * ACCEPT INPUT INFORMATION
   4.0020    AGAIN = 0
   4.0030    PRINT CR
   4.0040    PRINT 'LOCK-IN AMPLIFIER PHASE SETTINGS ARE CODED AS FOLLOWS:',CR
   4.0050    PRINT '          1. IN PHASE WITH BIAS PULSE',CR
   4.0060    PRINT '          2. 24.5 DEG BEFORE BIAS PULSE',CR
   4.0070    PRINT '          3. PHASE INDEPENDENT (VECTOR AMP OUTPUT)',CR
   4.0080    PRINT 'ENTER NUMBER FOR PHASE SETTING:'
   4.0090    IF(AGAIN) 4.012
   4.0100    ACCEPT PHAS
   4.0110    GO TO 4.015
   4.0120    ACCEPT CHANGE
   4.0130    IF(CHANGE EQ 0) 4.019
   4.0140    PHAS = CHANGE
   4.0150    IF(PHAS NE INT(PHAS)) 4.017
   4.0160    IF(1<PHAS<3) 4.019
   4.0170    PRINT 'TRY AGAIN',CR
   4.0180    GO TO 4.008
   4.0190    PRINT 'MATERIAL TYPES ARE CODED AS FOLLOWS:',CR
   4.0200    PRINT '        1. N-TYPE SILICON',CR
   4.0210    PRINT '        2. P-TYPE SILICON',CR
   4.0220    PRINT '        3. N-TYPE GALLIUM ARSENIDE',CR
   4.0230    PRINT '        4. P-TYPE GALLIUM ARSENIDE',CR
   4.0240    PRINT 'ENTER NUMBER FOR MATERIAL TYPE:'
```

```
4.0250   IF(AGAIN) 4.028
4.0260   ACCEPT MAT
4.0270   GO TO 4.031
4.0280   ACCEPT CHANGE
4.0290   IF(CHANGE EQ 0) 4.045
4.0300   MAT = CHANGE
4.0310   IF(MAT NE INT(MAT)) 4.033
4.0320   IF(1<MAT<4) 4.035
4.0330   PRINT 'TRY AGAIN',CR
4.0340   GO TO 4.024
4.0350   IF(MAT NE 1) 4.038
4.0360   C = C1
4.0370   GO TO 4.045
4.0380   IF(MAT NE 2) 4.041
4.0390   C = C2
4.0400   GO TO 4.045
4.0410   IF(MAT NE 3) 4.044
4.0420   C = C3
4.0430   GO TO 4.045
4.0440   C = C4
4.0450   PRINT 'DO YOU WANT POS. PEAKS (ENTER 1), NEG. PEAKS (ENTER -1),'
4.0460   PRINT CR,'OR BOTH (ENTER 0)?: '
4.0470   IF(AGAIN) 4.05
4.0480   ACCEPT YRANGE
4.0490   GO TO 4.056
4.0500   ACCEPT CHANGE
4.0510   IF(CHANGE EQ 0) 4.056
4.0520   IF(CHANGE NE 999) 4.055
4.0530   YRANGE=0
4.0540   GO TO 4.056
4.0550   YRANGE=CHANGE
4.0560   PRINT 'ENTER TEMP RANGE IN DEG KELVIN (25<T<350)',CR
4.0570   IF(AGAIN) 4.06
4.0580   ACCEPT 'TMIN=',TMIN
4.0590   GO TO 4.063
4.0600   ACCEPT 'TMIN=',CHANGE
4.0610   IF(CHANGE EQ 0) 4.069
4.0620   TMIN=CHANGE
4.0630   IF(25<TMIN<350) 4.066
4.0640   PRINT 'TEMP OUT OF RANGE 25<T<350',CR
4.0650   GO TO 4.057
4.0660   IF(AGAIN) 4.069
4.0670   ACCEPT 'TMAX=',TMAX
4.0680   GO TO 4.072
4.0690   ACCEPT 'TMAX=',CHANGE
4.0700   IF(CHANGE EQ 0) 4.081
4.0710   TMAX=CHANGE
4.0720   IF(TMAX LE 350)4.075
4.0730   PRINT 'TEMP OUT OF RANGE 25<T<350',CR
4.0740   GO TO 4.066
4.0750   IF(TMAX GT TMIN) 4.078
4.0760   PRINT 'TRY AGAIN',CR
4.0770   GO TO 4.056
4.0780   IF(AGAIN) 4.081
4.0790   ACCEPT 'WHAT IS THE LOCK-IN FREQUENCY?: ',F
4.0800   GO TO 4.086
4.0810   ACCEPT 'WHAT IS THE LOCK-IN FREQUENCY?: ',CHANGE
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    4.0820   IF(CHANGE EQ 0) 4.088
    4.0830   F=CHANGE
    4.0840   GO TO 4.088
    4.0850   IF(AGAIN) 4.088
    4.0860   ACCEPT 'HOW MANY PEAKS FOR THE COMBINED SPECTRUM?: ',N
    4.0870   GO TO 4.094
    4.0880   ACCEPT 'HOW MANY PEAKS FOR THE COMBINED SPECTRUM?: ',CHANGE
    4.0890   IF(CHANGE EQ 0) 4.094
    4.0900   IF(CHANGE NE 999) 4.093
    4.0910   N=0
    4.0920   GO TO 4.124
    4.0930   N=CHANGE
    4.0940   IF(1<N<10) 4.124,4.097,4.095
    4.0950   PRINT 'THAT'S A BIT MUCH',CR
    4.0960   GO TO 4.085
    4.0970   LOOP 4.123 J=1,N
    4.0980   PRINT CR
    4.0990   PRINT 'ENTER ACTIVATION ENERGY IN EV FOR PEAK ',J:IOC,': '
    4.1000   IF(AGAIN) 4.103
    4.1010   ACCEPT EC(J)
    4.1020   GO TO 4.106
    4.1030   ACCEPT CHANGE
    4.1040   IF(CHANGE EQ 0) 4.106
    4.1050   EC(J)=CHANGE
    4.1060   PRINT 'ENTER CROSS SECTION IN SQ CM FOR PEAK ',J:IOC,': '
    4.1070   IF(AGAIN) 4.11
    4.1080   ACCEPT SIGMAC(J)
    4.1090   GO TO 4.113
    4.1100   ACCEPT CHANGE
    4.1110   IF(CHANGE EQ 0) 4.113
    4.1120   SIGMAC(J)=CHANGE
    4.1130   PRINT 'ENTER AMPLITUDE (POS. OR NEG.) IN CM FOR PEAK ',J:IOC,': '
    4.1140   IF(AGAIN) 4.117
    4.1150   ACCEPT AMPC(J)
    4.1160   GO TO 4.123
    4.1170   ACCEPT CHANGE
    4.1180   IF(CHANGE EQ 0) 4.123
    4.1190   IF(CHANGE NE 999) 4.122
    4.1200   AMPC(J)=0
    4.1210   GO TO 4.123
    4.1220   AMPC(J)=CHANGE
    4.1230   CONTINUE
    4.1240   PRINT CR,'DO YOU WANT ANY PEAKS PLOTTED INDIVIDUALLY?',CR
    4.1250   IF (AGAIN) 4.128
    4.1260   ACCEPT 'IF SO, ENTER THE NUMBER; OTHERWISE HIT CR: ',NI
    4.1270   GO TO 4.134
    4.1280   ACCEPT 'IF SO, ENTER THE NUMBER; OTHERWISE ENTER 999: ',CHANGE
    4.1290   IF(CHANGE EQ 0) 4.134
    4.1300   IF(CHANGE NE 999) 4.133
    4.1310   NI=0
    4.1320   GO TO 5.01
    4.1330   NI=CHANGE
    4.1340   IF(1<NI<10) 5.01,4.137,4.135
    4.1350   PRINT 'THAT'S A BIT MUCH.',CR
    4.1360   GO TO 4.125
    4.1370   IF(N NE NI) 4.154
    4.1380   PRINT CR
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    4.1390    PRINT 'IF THESE ARE THE SAME PEAKS AS FOR THE COMBINED SPECTRUM,',CR
    4.1400    IF(AGAIN) 4.143
    4.1410    ACCEPT 'ENTER +1; OTHERWISE, HIT CR: ',SAME
    4.1420    GO TO 4.147
    4.1430    ACCEPT 'ENTER +1; OTHERWISE, ENTER 999: ',CHANGE
    4.1440    IF(CHANGE EQ 0) 4.147
    4.1450    IF(CHANGE EQ 999) 4.155
    4.1460    SAME=CHANGE
    4.1470    IF(SAME EQ 0) 4.155
    4.1480    LOOP 4.152 J=1,N
    4.1490    EI(J)=EC(J)
    4.1500    SIGMAI(J)=SIGMAC(J)
    4.1510    AMPI(J)=AMPC(J)
    4.1520    CONTINUE
    4.1530    GO TO 5.01
    4.1540    SAME=0
    4.1550    LOOP 4.181 J=1,NI
    4.1560    PRINT CR
    4.1570    PRINT 'ENTER ACTIVATION ENERGY IN EV FOR PEAK I-',J:IOC,': '
    4.1580    IF(AGAIN) 4.161
    4.1590    ACCEPT EI(J)
    4.1600    GO TO 4.164
    4.1610    ACCEPT CHANGE
    4.1620    IF(CHANGE EQ 0) 4.164
    4.1630    EI(J)=CHANGE
    4.1640    PRINT 'ENTER CROSS SECTION IN SQ CM FOR PEAK I-',J:IOC,': '
    4.1650    IF(AGAIN) 4.168
    4.1660    ACCEPT SIGMAI(J)
    4.1670    GO TO 4.171
    4.1680    ACCEPT CHANGE
    4.1690    IF(CHANGE EQ 0) 4.171
    4.1700    SIGMAI(J)=CHANGE
    4.1710    PRINT 'ENTER AMPLITUDE (POS. OR NEG.) IN CM FOR PEAK I-',J:IOC,': '
    4.1720    IF(AGAIN) 4.175
    4.1730    ACCEPT AMPI(J)
    4.1740    GO TO 4.181
    4.1750    ACCEPT CHANGE
    4.1760    IF(CHANGE EQ 0) 4.161
    4.1770    IF (CHANGE NE 999) 4.18
    4.1780    AMPI(J)=0
    4.1790    GO TO 4.181
    4.1800    AMPI(J)=CHANGE
    4.1810    CONTINUE

    5.0100 *  DRAW AXES
    5.0200    PRINT ERASE
    5.0300    VECTRF(40,780,40,110)
    5.0400    VECTRF(7,700,12,716)
    5.0500    VECTRF(12,716,17,700)
    5.0600    VECTRF(17,700,7,700)
    5.0700    CURSOR(21,700)
    5.0800    PRINT 'C'
    5.0900    VECTRF(40,110,1000,110)
    5.1000    VECTRF(1000,110,1000,780)
    5.1100    VECTRF(1000,780,40,780)
    5.1200    CURSOR(967,66)
    5.1300    PRINT 'TEMP'
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    6.0100 * DRAW SCALE ON HORIZONTAL AXIS
    6.0200   TMIN=INT(TMIN)
    6.0300   TMAX=INT(TMAX)
    6.0400   TK=TMAX
    6.0500   CALL 9.01
    6.0600   EMFMAX=EMF
    6.0700   TK=TMIN
    6.0800   CALL 9.01
    6.0900   EMFMIN=EMF
    6.1000   SCALE=(EMFMAX-EMFMIN)/70
    6.1100   DCOORD(EMFMIN-1.5*SCALE,EMFMAX,-22,4)
    6.1200   SCOORD(19,1000,88,114)
    6.1300   LOOP 6.21 TK=TMIN,TMAX
    6.1400   IF(TK/50 NE INT(TK/50))6.2
    6.1500   CALL 9.01
    6.1600   DRAWV(EMF,4,0)
    6.1700   DRAWV(EMF,-4,1)
    6.1800   DRAWV(EMF-1.5*SCALE,-22,-1)
    6.1900   PRINT TK:IOC
    6.2000   CONTINUE
    6.2100   CONTINUE
    6.2200   DRAWV(EMFMIN,0,0)

    7.0100 * CALCULATE AND DRAW DLTS SPECTRA
    7.0200 * ('SCALE' VALUES MUST BE ADJUSTED FOR HARD COPY IMAGE SIZE)
    7.0300   IF(PHAS NE 1) 7.06
    7.0400   SCALE = 2.31
    7.0500   GO TO 7.07
    7.0600   SCALE = 2.48
    7.0700   SCOORD(40,1000,110,780)
    7.0800   IF(YRANGE) 7.09,7.11,7.14
    7.0900   DCOORD(EMFMIN,EMFMAX,-SCALE,0)
    7.1000   GO TO 7.15
    7.1100   DCOORD(EMFMIN,EMFMAX,-SCALE/2,SCALE/2)
    7.1200   VECTRF(40,445,1000,445)
    7.1300   GO TO 7.15
    7.1400   DCOORD(EMFMIN,EMFMAX,0,SCALE)
    7.1500   IF(N LT 1) 7.31
    7.1600 * -COMBINED SPECTRUM
    7.1700   LOOP 7.21 J=1,N
    7.1800   E(J)=EC(J)
    7.1900   SIGMA(J)=SIGMAC(J)
    7.2000   AMP(J)=AMPC(J)
    7.2100   CONTINUE
    7.2200   LOOP 7.3 TK=TMIN,TMAX,.5
    7.2300   ASUM=0
    7.2400   LOOP 7.27 J=1,N
    7.2500   CALL 10.01
    7.2600   ASUM = ASUM+A
    7.2700   CONTINUE
    7.2800   CALL 9.01
    7.2900   DRAWV(EMF,ASUM,1)
    7.3000   CONTINUE
    7.3100   IF(NI LT 1) 8.01
    7.3200 * -INDIVIDUAL SPECTRA
    7.3300   LOOP 7.37 J=1,NI
    7.3400   E(J)=EI(J)
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   7.3500   SIGMA(J)=SIGMAI(J)
   7.3600   AMP(J)=AMPI(J)
   7.3700   CONTINUE
   7.3800   LOOP 7.49 J=1,NI
   7.3900   DRAWV(EMFMIN,0,0)
   7.4000   LOOP 7.48 TK=TMIN,TMAX,.5
   7.4100   CALL 10.01
   7.4200   CALL 9.01
   7.4300   IF(TK EQ INT(TK)) 7.46
   7.4400   DRAWV(EMF,A,1)
   7.4500   GO TO 7.47
   7.4600   DRAWV(EMF,A,0)
   7.4700   CONTINUE
   7.4800   CONTINUE
   7.4900   CONTINUE

   8.0100 * PRINT INPUT INFO
   8.0200   CURSOR(770,44)
   8.0300   IF(MAT NE 1) 8.06
   8.0400   PRINT 'N-SI'
   8.0500   GO TO 8.13
   8.0600   IF(MAT NE 2) 8.09
   8.0700   PRINT 'P-SI'
   8.0800   GO TO 8.13
   8.0900   IF(MAT NE 3) 8.12
   8.1000   PRINT 'N-GAAS'
   8.1100   GO TO 8.13
   8.1200   PRINT 'P-GAAS'
   8.1300   IF(PHAS NE 1) 8.16
   8.1400   PRINT ' (0 DEG)'
   8.1500   GO TO 8.2
   8.1600   IF(PHAS NE 2) 8.19
   8.1700   PRINT ' (24.5 DEG)'
   8.1800   GO TO 8.2
   8.1900   PRINT ' (PH IND)'
   8.2000   CURSOR(714,22)
   8.2100   PRINT F:R1,'HZ'
   8.2200   CURSOR(742,0)
   8.2300   PRINT TMIN:IO,'< T < ',TMAX:IOC
   8.2400   CURSOR(0,44)
   8.2500   IF(N EQ 0) 8.3
   8.2600   LOOP 8.29 J=1,N
   8.2700   PRINT 'PEAK ',J:IOC,':^H',EC(J):R3C,' EV; ',SIGMAC(J):E2C
   8.2800   PRINT ' SQ CM; AMPL=',AMPC(J):F3C,'CM',CR
   8.2900   CONTINUE
   8.3000   IF(NI EQ 0) 8.36
   8.3100   IF(SAME EQ 1) 8.36
   8.3200   LOOP 8.35 J=1,NI
   8.3300   PRINT 'PEAK I-',J:IOC,':^H',EI(J):R3C,' EV; ',SIGMAI(J):E2C
   8.3400   PRINT ' SQ CM; AMPL=',AMPI(J):F3C,'CM',CR
   8.3500   CONTINUE
   8.3600   PRINT CR,CR
   8.3700   GO TO 11.01

   9.0100 * CALCULATION OF APPROXIMATE!! EMF AS FUNCTION OF T
   9.0200 *   (SEE 'TEMPERATURE, ITS MEAS & CTRL IN SCI & IND,' VOL 4, PT 3,
   9.0300 *   ED. H.H.PLUMB (PITTSBURG,1972), PG. 1613.)
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   9.0400    TC=TK-273
   9.0500    I=2
   9.0600    IF(TC LT X(3))9.09
   9.0700    I=3
   9.0800    GO TO 9.13
   9.0900    IF(TC-X(I)) 9.12,9.13,9.1
   9.1000    I=I+1
   9.1100    GO TO 9.09
   9.1200    I=I-1
   9.1300    HT1=TC-X(I)
   9.1400    HT2=TC-X(I+1)
   9.1500    PROD=HT1*HT2
   9.1600    H=X(I+1)-X(I)
   9.1700    DELY=(Y(I+1)-Y(I))/H
   9.1800    S3=(S2(I+1)-S2(I))/H
   9.1900    SS2=S2(I)+HT1*S3
   9.2000    DELSQS=(S2(I)+S2(I+1)+SS2)/6
   9.2100    EMF=Y(I)+HT1*DELY+PROD*DELSQS
   9.2200    RETURN

  10.0100 * CALCULATION OF DLTS CURVE AMPLITUDE
  10.0200 * ('IF' STATEMENTS AVOID EXCEEDING RANGE OF 10**-38 TO 10**+38)
  10.0300    IF(E(J)/(K*TK) LT 86) 10.06
  10.0400    A=0
  10.0500    GO TO 10.17
  10.0600    POWR1=EXP(E(J)/(K*TK))
  10.0700    ALPHA=F*C*POWR1/(SIGMA(J)*TK**2)
  10.0800    IF(ALPHA GT .013) 10.11
  10.0900    POWR2=0
  10.1000    GO TO 10.15
  10.1100    POWR2=EXP(-1/ALPHA)
  10.1200    IF(E(J)/(K*TK) LT 43) 10.15
  10.1300    A1=AMP(J)*2*(1-POWR2)/PI**2
  10.1400    GO TO 10.19
  10.1500    IF(PHAS NE 1) 10.18
  10.1600    A = AMP(J)*8*ALPHA**2*(1-POWR2)/(4*PI**2*ALPHA**2+1)
  10.1700    GO TO 10.23
  10.1800    A1 = AMP(J)*4*ALPHA*(1-POWR2)/(PI*SQRT(4*PI**2*ALPHA**2+1))
  10.1900    IF(PHAS NE 2) 10.22
  10.2000    A = A1*COS(ATAN(1/(2*PI*ALPHA))-PHASE)
  10.2100    GO TO 10.23
  10.2200    A = A1
  10.2300    RETURN

  11.0100 * ALLOW REPEAT WITH SOME INPUT INFO CHANGED
  11.0200    PRINT 'IF YOU WANT A REPEAT WITH SOME INPUT DATA CHANGED,',CR
  11.0300    ACCEPT 'HIT CR; OTHERWISE ENTER 1:', REPT
  11.0400    IF(REPT NE 0) 11.11
  11.0500    PRINT CR,'AS INPUT DATA IS REQUESTED, IF YOU WISH THAT QUANTITY',CR
  11.0600    PRINT 'UNCHANGED, SIMPLY HIT CR.',CR
  11.0700    PRINT '(NOTE:  TO CHANGE A NON-ZERO VALUE TO ZERO, YOU MUST',CR
  11.0800    PRINT 'ENTER 999.)',CR
  11.0900    AGAIN=REPT+1
  11.1000    GO TO 4.003
  11.1100    STOP
```